A STRATEGY FOR DETECTING EXTREME EIGENVALUES BOUNDING GAPS IN THE DISCRETE SPECTRUM OF SELF-ADJOINT OPERATORS *

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Abstract. For a self-adjoint linear operator with discrete spectrum or a Hermitian matrix the "extreme" eigenvalues define the boundaries of clusters in the spectrum of real eigenvalues. The *outer* extreme ones are the largest and the smallest eigenvalues. If there are extended intervals in the spectrum in which no eigenvalues are present, the eigenvalues bounding these gaps are the *inner* extreme eigenvalues.

We will describe a procedure for detecting the extreme eigenvalues that relies on the relationship between the acceleration rate of polynomial acceleration iteration and the norm of the matrix via the spectral theorem, applicable to normal matrices. The strategy makes use of the fast growth rate of Chebyshev polynomials to distinguish ranges in the spectrum of the matrix which are devoid of eigenvalues.

The method is numerically stable with regard to the dimension of the matrix problem and thus capable of handling matrices of large dimension. The overall computational cost is quadratic in the size of a dense matrix; linear in the size of a sparse matrix. We verify computationally that the algorithm is accurate and efficient, even on large matrices.

Key words. eigenvalues, spectral gaps, accelerated convergence, Hermitian matrix.

AMS subject classifications. 15A15, 15A09, 15A23

1. Introduction.

We present an accurate and efficient application of polynomials to determine "extreme" eigenvalues of a Hermitian matrix $M = I - A$. Here A and I are $m \times m$, the latter being the identity matrix. The strategy applies in a straightforward way to the more general problem of finding the extreme eigenvalues of self adjoint linear operators. This linear operator may be available to us in matrix form, but more generally it can be presented to us in some less explicit form, or perhaps operationally, as a computer routine or set of instructions which can be taken as a black box input to the extreme eigenvalue strategy to be presented. We develop the strategy for the Hermitian matrix case, as the manner in which extreme eigenvalues of the linear operator case are obtained is identical to the matrix case.

The *outer extreme eigenvalues* are defined as the smallest and largest ones bounding the smallest interval containing all the eigenvalues of M.

If, in addition, the eigenvalues of M are clustered, then there are gaps in the spectrum. We denote the eigenvalues defining the gaps and that are not outer extreme eigenvalues as the *inner extreme eigenvalues*.

Figure 1.1 illustrates the eigenvalue distribution of a matrix M which has both outer and inner extreme eigenvalues. In the figure the inner extreme eigenvalues are a' and b', defining in this case a single gap in the spectrum. Generality is not lost by assuming that the eigenvalues of M are entirely contained in the interval $(-1, 1)$ –the

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original matrix might need to be multiplied by a scaling factor for this condition to hold–.

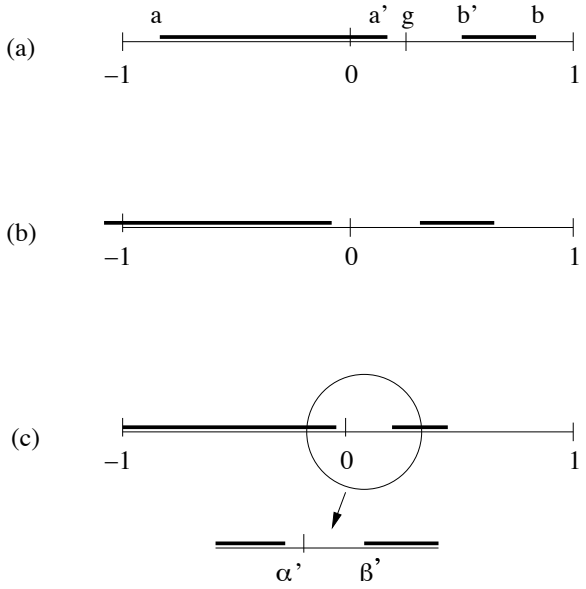

FIG. 1.1. *(a) Schematic of the spectrum of M and the location of the extreme eigenvalues, with a and b corresponding to the outer ones and a' and b' being the inner ones, $(a < a' < b' < b)$. M can have many inner extreme eigenvalues and their location need not determined by equal intervals. The extreme eigenvalues of A are implied by the relation $M = I - A$. (b) Shifted matrix $M - gI$. (c) Shifted and scaled matrix $(M - gI)/\lambda$; $\lambda = \max(|a - g|, |b - g|)$.*

The interplay between approximation theory and numerical linear algebra has a long history (see [1], [2], [3] [4], [5], [6], [7]). Chebyshev iteration exploits the optimality rpoperties of Chebyshev polynomials to iteratively solve linear systems of equations [8], [9].

The determination of *clusters* of eigenvalues is particularly important in applications such as computational chemistry [10]. In many problems in chemistry and physics involving matrices with clustered eigenvalues an estimate of the interval defining the larger cluster is of great interest: for example, Gear and Kevrekidis [11] propose a numerical integration scheme which is ideally suited to evolution problems with multiscale behavior. This multiscale behavior arises because there is a clear separation in the distribution of the eigenvalues associated with the evolution operator. The integration scheme relies on knowing where to split the spectrum of the evolution operator. In a totally different realm, another application of our strategy would be in the accurate determination of the extreme eigenvalues of a matrix with clustered eigenvalues. Accurate estimates of the extreme eigenvalues can then be exploited in building a matrix polynomial preconditioner to the given Hermitian matrix [12].

Finding the outer extreme eigenvalues, particularly when Hermitian matrices are involved, is a straightforward application of the power method or Rayleigh Ritz, for example. Some of the more effective strategies for finding clusters of eigenvalues are related to the Lanczos method, particularly when large matrices are involved. Methods for finding a *few* eigenvalues, usually located near a given eigenvalue, are also available (see for example [13]). Here we present an algebraic strategy that exploits polynomial interpolation to specifically target the determination of the gaps

in the spectrum of the operator or matrix, and in this sense it is novel.

Our methodology is capable of estimating the inner extreme eigenvalues accurately and efficiently; the accuracy will be demonstrated by numerical examples. The computational cost of the proposed extreme eigenvalue estimation methodology is dominated by the matrix-vector multiplies. This cost ranges from $\mathcal{O}(m^2)$ for a dense $m \times m$ matrix and $\mathcal{O}(m)$ for sparse matrices. This estimate of the complexity of the algorithm is obtained as follows (in the dense case): each step of the iteration process (3.1) has a cost of m^2 operations.

We estimate the extreme eigenvalues of the matrix $Ax = q$ by a technique that we call "reverse Chebyshev acceleration" (RCA). For a Hermitian matrix the spectral theorem gives us a sharp bound on the norm of the matrix in terms of its eigenvalues. The rate of convergence of an iterative Chebyshev linear solver can be estimated using this bound; if we knew the spectrum of the matrix we could obtain an optimal rate of convergence in the implementation of the solver. Here we use this fact to obtain the unknown extreme eigenvalues by iteratively improving on an initial guess of the extreme eigenvalues, we start with a vector x and a right hand side vector q, that satisfy the equality $q = Ax$. An algorithmic strategy that determines the degree of "misfit" of successive guesses to the location of the extreme eigenvalues: the extent to which the acceleration of convergence of the iterative method differs from the acceleration that one would witness if all the eigenvalues of $M = I - A$ were indeed located in the guessed intervals indicates the extent to which a successive guess of the location of the extreme eigenvalues must be modified by to contain all the eigenvalues. The strategy, though fundamentally inspired by an iterative procedure, can be made significantly more efficient: as we will see, the iteration can be side-stepped entirely and reduced to solving a single equation. The computational cost will then be entirely related to matrix-vector multiplies, $\mathcal{O}(m^2)$ operations for dense matrices.

The RCA strategies for finding the outer and the inner extreme eigenvalues are slightly different: the outer extreme case will use an extremal polynomial for one interval of the real line, while the inner extreme case will employ an extremal polynomial, constructed specifically over two disjoint intervals. As mentioned before, the outer extreme eigenvalues may be found by conventional means, hence our consideration of finding these with the proposed strategy is mostly motivated by didactic considerations, that is, by first considering this case, it makes it significantly easier to understand how the inner extreme eigenvalues will be found.

We focus here on arbitrary Hermitian matrices, *i.e.*, dense or otherwise. However, the procedure generalizes to the consideration of arbitrary normal matrices, in which case the problem of finding extreme eigenvalus would be: Given a matrix A, with possibly complex eigenvalue spectrum $Sp(A)$, find a curve Γ "enclosing closely" $Sp(A)$. If the strategy is to be viable, we want to determine this curve in at most $\mathcal{O}(m^2)$ steps. The main ingredient in building the curve Γ is the family of *Faber* polynomials [14]. These reduce to Chebyshev polynomials when Γ is a line in the complex plane, the case under consideration in this paper. Among their properties, extremal polynomials, such as Chebyshev polynomials, grow extremely fast outside the unit interval. (See [14], [15] for further information).

2. Extremal Property of the Chebyshev Polynomials. The Chebyshev polynomials $T_n(z)$ are the fastest growing polynomials, for $|z| \geq 1$ (see [16]). These polynomials satisfy the property $T_n(\cos\ \theta) = \cos(n\ \theta), \quad \cos\ \theta = z$, for, $z \in \mathbb{R}$, and

hence

$$T_n\left(\frac{1}{2}\left(z+\frac{1}{z}\right)\right)=\frac{1}{2}\left(z^n+\frac{1}{z^n}\right),\quad z\neq 0. \tag{2.1}$$

The extremal property of fundamental importance to the detection of eigenvalues of a matrix is the following:

THEOREM 2.1. *Let $P_n(z)$ be a polynomial of degree (at most) n with the following property*

$$\sup_{x\in[-1,1]}|P_n(z)|\leq 1. \tag{2.2}$$

Let $z\in\mathbb{R}$ with $|z|>1$. Then

$$|P_n(z)|\leq|T_n(z)|.$$

Moreover if equality is achieved above then

$$P_n(z)=\pm T_n(z).$$

□

Thus, it is not possible to find $P_n(z)$ satisfying (2.2) with $|P_n(z)|>\frac{1}{2}\left(\left(|z|+\sqrt{z^2-1}\right)^n+\left(|z|-\sqrt{z^2-1}\right)^n\right)$, for $|z|>1$.

The reason why we prefer to use (2.1) instead of direct evaluation of $T_n(z)$ is that (2.1) yields estimates of the rate of growth of $|T_n(z)|$ for $z\notin[-1,1]$. If $z>1$, then $T_n(z)=\frac{1}{2}\left(\alpha^n+\alpha^{-n}\right)$, where $\alpha=z+\sqrt{z^2-1}$. More generally let $z\in\mathbb{R}$, $z\notin[-1,1]$ and let $\alpha>1$ solve $|z-1|+|z+1|=\alpha+\alpha^{-1}$. Then $\frac{1}{2}\left(\alpha^n+\alpha^{-n}\right)\geq|T_n(z)|\geq\frac{1}{2}\left(\alpha^n-\alpha^{-n}\right)$. When the interval $[-1,1]$ is replaced by $[a,b]$, where $a<b$ (see Figure 1.1), the Chebyshev polynomials take the form

$$P_n^{a,b}(z):=T_n\left(\frac{2z}{b-a}-\frac{b+a}{b-a}\right).$$

2.1. An Extreme Polynomial Defined On Two Disjoint Intervals. The determination of the inner extreme eigenvalues is made possible by the proposed new extreme polynomial for the union of two intervals $[-b,-a]\cup[a,b]$.

THEOREM 2.2. *Let $0<a<b$, and define*

$$\mathcal{P}_{2n}^{a,b}(z):=T_n\left(\frac{2z^2}{b^2-a^2}-\frac{b^2+a^2}{b^2-a^2}\right) \tag{2.3}$$

for $z\in\mathbb{R}$ with $z\notin[-b,-a]\cup[a,b]$. Let $\mathcal{Q}_{2n}(z)$ be an even polynomial with the property that

$$\sup_{z\in[-b,-a]\cup[a,b]}|\mathcal{Q}_{2n}^{a,b}(z)|\leq 1.$$

Then

$$|\mathcal{Q}_{2n}^{a,b}(z)|\leq|\mathcal{P}_{2n}^{a,b}(z)|.$$

Proof. Because $\mathcal{Q}_{2n}(z)$ is even, it is possible to find a polynomial $R_n(z)$ of degree n with

$$\mathcal{Q}_{2n}(z)=R_n\left(\frac{2z^2}{b^2-a^2}-\frac{b^2+a^2}{b^2-a^2}\right). \tag{2.4}$$

The polynomials

$$\left(\left(\frac{2z^2}{b^2-a^2}-\frac{b^2+a^2}{b^2-a^2}\right)^k\right)_{k=0}^{n}$$

form a linearly independent set of $n+1$ even polynomials of degree $2k$, $k=0,\ 1,\ \cdots,\ n$. Hence this set spans all even polynomials of degree at most $2n$.

Let z^0 be a specific value of z and define

$$y^0=\frac{2(z^0)^2}{b^2-a^2}-\frac{b^2+a^2}{b^2-a^2}.$$

Then $|y^0|>1$ because for $z\in[-b,-a]\cup[a,b]$, we have $\frac{2z^2}{b^2-a^2}-\frac{b^2+a^2}{b^2-a^2}\in[-1,1]$. Using Theorem 2.1 and (2.4) we have

$$|T_n(y^0)|\geq|R_n(y^0)|=|\mathcal{Q}_{2n}(z^0)|,$$

and in view of (2.3) it follows that

$$T_n(y^0)=\mathcal{P}_{2n}^{a,b}(z^0).$$

□

Theorems 2.1 and 2.2 play crucial roles in the reverse acceleration of convergence to detect extreme eigenvalues (see Section 4 and Appendix A).

3. Review of the Polynomial Acceleration Technique. The classical acceleration technique, for the iterative solution of the linear system $Ax=q$, will be used to find extreme eigenvalues. We do this by exploiting the relation between the acceleration rate to the spectrum of the matrix (via the spectral theorem), optimized via extremal polynomials, to estimate the location of the extreme eigenvalues via a systematic seach algorithm.

We begin by reviewing the theory for accelerating iterative methods for solving linear systems. Let A be an invertible matrix of size m and define

$$M=I-A,$$

where I is the $m\times m$ identity matrix. Assume, moreover, that the eigenvalues of M are all less than 1 in absolute value. The iteration scheme

$$x_{k+1}=Mx_k+q,\quad k=0,1,2,\ldots, \tag{3.1}$$

with a given initial guess x_0 converges to the solution x of $Ax=q$. The error $e_k=x_k-x$ at the k^{th} step, satisfies $e_k=M^ke_0$.

The iteration can be accelerated by defining parameters $\gamma_0,\ \gamma_1,\ldots,\gamma_n\in\mathbb{R}$, with $\sum_{k=0}^{n}\gamma_k=1$, such that a linear combination of past iterates

$$y_n:=\sum_{k=0}^{n}\gamma_kx_k, \tag{3.2}$$

satisfies

$$\|y_n-x\|\ll\|x_n-x\|. \tag{3.3}$$

Using (3.2) we can thus surmise

$$y_n - x = \sum_{k=0}^{n} \gamma_k M^k e_0,$$

and

$$\|y_n - x\| \leq \left\| \sum_{k=0}^{n} \gamma_k M^k \right\| \|e_0\|. \tag{3.4}$$

Define

$$P_n(z) := \sum_{k=0}^{n} \gamma_k z^k. \tag{3.5}$$

Then

$$\|y_n - x\| \leq ||P_n(M)|| \, \|e_0\| = \sup_{z \in S_p(M)} |P_n(z)| \, \|e_0\|, \tag{3.6}$$

where Sp denotes "the spectrum of," provided A (and thereby M) is normal, since for such matrices

$$\|P_n(A)\| = \sup_{z \in Sp(A)} |P_n(z)|.$$

Hence the acceleration of convergence of the iterative scheme (3.1), using (3.2), will be achieved if the coefficients $\gamma_0,\ \gamma_1, \cdots, \gamma_n$ are such that $P_n(1) = 1$, and the *minimax property*, where

$$\sup_{z \in S_p(M)} |P_n(z)| \quad \text{is minimized}$$

holds. The extremal properties of the Chebyshev polynomials make them good candidates for solving the minimax problem.

4. Localization of the Inner Extreme Eigenvalues. Determination of the outer extreme eigenvalues for a Hermitian matrix is easily accomplished by the power method. In what follows it will be assumed that these eigenvalues, and the eigenfunction associated with the largest eigenvalue are known. Nevertheless, our strategy can be used to find the outer extreme eigenvalues, and for completeness, the strategy that applies to this case appears in Appendix A.

The accurate and efficient estimation of the inner eigenvalues is where our approach is particularly effective and useful, since there are no well-known methods that can make this estimate accurately in $\mathcal{O}(m^2)$ operations for dense normal matrices.

We assume that for the Hermitian matrix M we have $S_p(M) \subset (-1, 1)$. This latter condition can always be satisfied by scaling M as shown in Figure 1.1. We pick an x and thus determine $q = Ax$ explicitly. We require that the initial iterate eigenvector x_0 be associated with the eigenvalue of largest absolute value of $P_n(M)$. Again, this is found by the power method in at most $\mathcal{O}(m^2)$ operations. The initial error e_0 is defined once the eigenvector x_0 is known.

The localization strategy which we call *reverse Chebyshev acceleration* (RCA), uses the extremal polynomial $\tilde{\mathcal{P}}_{2n}^{a,b}(x)$. It is part of the larger strategy of finding all of the inner extreme eigenvalues.

4.1. RCA Preliminaries. For the integer $n \geq 1$, and for $0 < s < \beta < 1$, we denote

$$\tilde{\mathcal{P}}_{2n}^{s,\beta}(x) := \frac{\mathcal{P}_{2n}^{s,\beta}(x)}{\mathcal{P}_{2n}^{s,\beta}(1)}. \tag{4.1}$$

Note that $\tilde{\mathcal{P}}_{2n}^{s,\beta}(x)$ is a polynomial of degree $2n$. As in the setting of Subsection A the analogue of Theorem A.1 is now

THEOREM 4.1. *Let β and s be as above. Let the first guess x_0 be the eigenfunction corresponding to the largest eigenvalue, in absolute terms, of $\mathcal{P}_{2n}^{s,\beta}(M) = \sum_{k=0}^{2n} \gamma_k M^k$. Let*

$$y_{2n} := \sum_{k=0}^{2n} \gamma_k x_k,$$

where the coefficients γ_k are those of $\tilde{\mathcal{P}}_{2n}^{s,\beta}(x)$ given above. Then all the eigenvalues of M are located in $[-\beta, -s] \cup [s, \beta]$ if and only if

$$\|y_{2n} - x\| = \sup_{x \in [-\beta,-s]\cup[s,\beta]} |\tilde{\mathcal{P}}_{2n}^{s,\beta}(x)| \, \|e_0\|. \tag{4.2}$$

The proof follows the same lines as those of the proof of Theorem A.1 and is therefore omitted. □

The analogue of Theorem A.2 in the present setting is

THEOREM 4.2. *Let $0 \leq s < \beta < 1$. Let the first guess x_0 be the eigenfunction corresponding to the largest eigenvalue, in absolute value, of M. Define e_0 in terms of x_0. Assume, with the notations of Theorem 4.1, that*

$$\|y_{2n} - x\| > \sup_{x \in [-\beta,-s]\cup[s,\beta]} \tilde{\mathcal{P}}_{2n}^{s,\beta}(x)| \, \|e_0\|. \tag{4.3}$$

Then there is at least one eigenvalue λ of M in $(-s, s)$ and an estimate of the eigenvalue closest to zero is solution of the following equation:

$$\left|\tilde{\mathcal{P}}_{2n}^{s,\beta}(\eta)\right| = \frac{\|y_{2n} - x\|}{\|e_0\|}. \tag{4.4}$$

Again the proof is similar to that of Theorem A.2. □

The last results on which our algorithm will be based is

PROPOSITION 4.1. *If*

$$\|y_{2n} - x\| = \sup_{x \in [-\beta,\beta]} |\mathcal{P}_{2n}^{s,\beta}(x)| \, \|e_0\| \tag{4.5}$$

then 0 is an eigenvalue of M. Proof. The proof follows at once from the fact that

$$|\mathcal{P}_{2n}^{s,\beta}(0)| = \sup_{x \in [-\beta,\beta]} |\mathcal{P}_{2n}^{s,\beta}(x)|.$$

□

COROLARY 4.1. *If 0 is not an eigenvalue of M then*

$$\|y_{2n} - x\| < \sup_{x \in [-\beta,\beta]} |\tilde{\mathcal{P}}_{2n}^{s,\beta}(x)| \, \|e_0\| \tag{4.6}$$

Let δ denote an arbitrary real number, and η be the x real values that satisfy

$$\left|\mathcal{P}_{2n}^{s,\beta}(x)\right| = \left|T_n\left(\frac{2x^2}{\beta^2 - s^2} - \frac{\beta^2 + s^2}{\beta^2 - s^2}\right)\right| = \delta, \quad \delta > 1.$$

Specifically, these are

$$\eta = \pm\sqrt{\pm\frac{1}{2}(\beta^2 - s^2)\tilde{y} + \frac{1}{2}(\beta^2 + s^2)} \tag{4.7}$$

with, as in (A.9),

$$\tilde{y} = \frac{1}{2}\left(\left(\delta + \sqrt{\delta^2 - 1}\right)^{\frac{1}{n}} + \left(\delta - \sqrt{\delta^2 - 1}\right)^{\frac{1}{n}}\right). \tag{4.8}$$

Notice that if

$$\delta > T_n\left(\frac{\beta^2 + s^2}{\beta^2 - s^2}\right) \tag{4.9}$$

then there are only two real solutions, whose absolute values are greater than β, namely,

$$\eta = \pm\sqrt{\frac{1}{2}(\beta^2 - s^2)\tilde{y} + \frac{1}{2}(\beta^2 + s^2)}. \tag{4.10}$$

On the other hand if

$$1 < \delta \leq T_n\left(\frac{\beta^2 + s^2}{\beta^2 - s^2}\right)$$

exactly two of the four (real) solutions are located in $[-s, s]$. Namely

$$\eta = \pm\sqrt{-\frac{1}{2}(\beta^2 - s^2)\tilde{y} + \frac{1}{2}(\beta^2 + s^2)} \tag{4.11}$$

with $\tilde{y}$ as above. Now let δ take the specific value

$$\delta = \frac{\|y_{2n} - x\|}{\|e_0\|}\mathcal{P}_{2n}^{s,\beta}(1). \tag{4.12}$$

We illustrate key aspects of the algorithm in Figure 4.1. In this example $|a| = |b| := b$, and there is one gap in the spectrum with $|a'| = |b'| := a'$. Suppose we guess that the eigenvalues of M are located in $[-1, -s] \cup [s, 1]$. $(0 < s < 1.)$ If this assumption was correct then the above algorithm tells us that we would witness an acceleration of convergence equal to $\mathcal{P}_8(s)$, the height of the lower horizontal line above the $x-$axis in the figure. However if the true (i.e., observed) acceleration of convergence is δ, with $\delta > \mathcal{P}_8(s)$ as is the case here, the above algorithm tells us that the eigenvalues of M are located in $[-1, -a'] \cup [a', 1]$ where a' is such that $\mathcal{P}_8(a') = \delta$. The value of a' that must be chosen is such that $0 < a' < 1$. Morever, as is implied by the algorithm, this value of a' is optimal in the sense that if $t' > a'$ (and $t' < 1$) then there are eigenvalues of M located in $[a', t']$ or $[-t', -a']$.

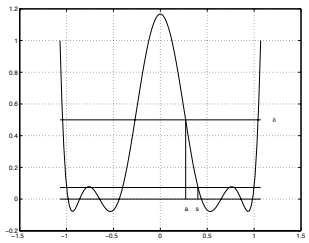

FIG. 4.1. *Plot of* $\mathcal{P}_8^{a'=0.4,b=1}$, *as given by (2.3), with* s *and* δ *as described in the text. The height of the horizontal line above the x-axis is* $\mathcal{P}_8(s)$.

4.2. The Algorithm. We assume that we already know the outer extremal eigenvalues a and b, by the power method (or using the procedure outlined in Appendix A). The algorithm first shifts and scales the operator to "place" the targeted gap with associated inner extremal eigenvalues close to the origin (see Figure 1.1). The shift is of the form $M - gI$, where g is a point in the gap. A scaling is required so that the eigenvalues of $M - gI$ remain within the interval $[-1, 1]$. To find the inner extreme eigenvalues we require initial guesses g_i, $i = 1, 2.., K$, where K is the number of gaps in the spectrum of M. Each g_i is chosen so as to place the zero value in one of the gaps of M. RCA is then used to find the pair of inner extreme eigenvalues a_i' and b_i' associated with each g_i.

The steps for identifying the first gap are:

1. *scale and shift*: shift and scale the matrix, so that we obtain

$$(M - g_1 I)/\lambda_1,$$

   where $\lambda_1 = max(|a - g_1|, |b - g_1|)$, as shown in Figure 1.1:.
2. *finding the closest inner eigenvalue*: apply the RCA algorithm (see below) to find the distance σ between g_1 and the closest extreme eigenvalue. It could be $\alpha_1 = (a_1' - g_1)/\lambda_1$ or $\beta_1 = (b_1' - g_1)/\lambda_1$. The outer extreme eigenvalues in the scaled-shifted matrix are now α and β.
3. *determining whether the closest eigenvalue is* α_1 *or* β_1: shift and scale the matrix to obtain

$$(M - (g_1 + \sigma)I)/\lambda_\sigma,$$

   where $\lambda_\sigma = max(|a - g_1 - \sigma|, |b - g_1 - \sigma|)$. If (4.5) holds,

$$\beta_1 = (g_1 + \sigma)/\lambda_\sigma,$$

   otherwise,

$$\alpha_1 = (g_1 - \sigma)/\lambda_\sigma.$$

4. *finding the other inner extreme eigenvalue*: if $\beta_1 = (g_1 + \sigma)/\lambda_\sigma$, we find α_1 as follows: shift and scale

$$(M - (g_1 - 2\sigma)I)/\lambda^+_{2\sigma},$$

where $\lambda^+_{2\sigma} = max(|a - g_1 + 2\sigma|, |b - g_1 + 2\sigma|)$, and apply the RCA algorithm to this matrix.
if $\alpha_1 = (g_1 - \sigma)/\lambda_\sigma$, we find β_1 as follows: shift and scale

$$(M - (g_1 + 2\sigma)I)/\lambda^-_{2\sigma},$$

where $\lambda^-_{2\sigma} = max(|a - g_1 - 2\sigma|, |b - g_1 - 2\sigma|)$, and apply the RCA algorithm to this matrix.

To find a'_2 and b'_2 the procedure 1-4 is repeated with g_1, α_1, β_1 replaced by g_2, α_2, β_2, and so on.

4.2.1. The RCA Algorithm.

1. We make a guess s for σ $(0 < s < \beta)$. If (4.2) holds then all the eigenvalues of M are $[-\beta, -s] \cup [s, \beta]$,. There are no eigenvalues in $[-s, s]$.
2. Choose $s < s' < \beta$ and replace $s \leftarrow s'$. If (4.3) holds it must be the case that some eigenvalues of M are contained $(-\alpha', \alpha')$.
3. Compute η using using (4.12), (4.8) and (4.11). and put $s \leftarrow |\eta|$. The resulting s is an estimate, to within machine accuracy, of σ.

5. Numerical Results. We consider two types of problems to demonstrate that the proposed algorithm is numerically robust, accurate, and computationally effective, especially when the matrix dimension is large. In one example we apply the algorithm on a matrix for which the spectrum is poorly distributed. The second example is one in which the eigenvalues are evenly distributed in $[a, a'] \cup [b', b]$. Here, the gap is simply the interval between the inner extreme eigenvalues a' to b' (see Figure 1.1). Although making the clusters symmetric about zero is inconsequential to the success of the algorithms, both cases presented below use matrices with an eigenvalue spectrum wholly contained in the range $[-0.8, -0.6]$ and $[0.6, 0.8]$. In the examples that follow the number of Chebyshev coefficients used is fixed at $n = 13$.

We will assume that the outer extremal eigenvalues are known (obtained via the the power method). We then proceed to determine the gap in the spectrum, *i.e.*, the inner extreme eigenvalues. We will test the algorithm on two types of problems. We will denote as *problem I* that of finding the gap to a family of normal matrices with well distributed eigenvalues. These are matrices that are constructed to have a fixed size gap and that, as the size of the matrix is made larger, contain more eigenvalues in the non-gap range. Furthermore, their distribution is uniform outside of the gap. Thus, for the matrix of size 4, the eigenvalues are $-0.8, -0.6, 0.6, 0.8$; for the matrix of size 10, the eigenvalues are $-0.8, -0.75, -0.7, -0.65, -0.6, 0.6, 0.65, 0.7, 0.75, 0.8$, and so on. A matrix with this spectrum can be generated by the following procedure: Find an orthogonal matrix Q by performing a QR decomposition of a random matrix of size m. Construct a diagonal matrix D of size m with entries equal to the eigenvalues. Then, the matrix $B = Q^\dagger DQ$ will result in a matrix of size m with the eigenvalues corresponding to the non-zero entries in D.

Table 5.1 gives the relative error between the estimate and the exact value of positive inner extreme eigenvalue as a function of the matrix size m. As the table suggests, our estimate of the eigenvalue is very accurate. Moreover, the estimate of

TABLE 5.1

Relative error between the estimate of the gap and its true value as a function of matrix size m, for matrix problem I The matrix corresponding to problem I has a uniform distribution of eigenvalues in its spectrum (see text). The exact gap spans -0.6 to 0.6.

m	relative error
6	1.870171e-12
10	6.698346e-13
18	4.946044e-13
34	1.028807e-13
66	4.303224e-12
130	8.992806e-14
162	1.191639e-12
322	1.313764e-13

the value does not deteriorate with matrix size and thus appears to be numerically stable with regard to matrix size.

Table 5.2 considers a family of matrices that have poorly distributed eigenvalues. This example will be denoted as *problem II*. In this case we constructed matrices for which the degenerate eigenvalues are $-0.8, -0.6, 0.6$, and 0.8. The circulant matrix is constructed by applying a discrete Fourier transform to a vector with entries equal to the eigenvalues. The matrix so constructed will possess the four eigenvalues just mentioned, with multiplicity $m/4$, where m is chosen commensurate to 4. In other words, the matrix of size 4 will be build to contain the eigenvalues $-0.8, -0.6, 0.6, 0.8$; the matrix of size 8 will contain $-0.8, -0.8, -0.6, 0.6, 0.6, 0.6, 0.8, 0.8$, and so on.

TABLE 5.2

Relative error between the estimate of the gap and its true value as a function of matrix size m, for problem II. The circulant matrices have degenerate eigenvalues, and a gap that spans -0.6 to 0.6. See text.

m	relative error
4	2.368291e-12
8	1.483998e-13
16	3.811766e-14
32	1.229387e-12
64	1.529517e-12
128	6.032212e-14
256	1.852222e-13

The efficacy and the convergence rate might be expected to degrade in problem II due to the uneven distribution of the eigenvalues outside of the gap. The lack of uniformity in the distribution of the eigenvalues makes the acceleration norm larger as compared to its value in the gap region. However, no significant deterioration is evident in the results reported in the table, as evidenced in Table 5.2.

These numerical examples suggest that the algorithms are robust and practical; they do not show any evidence of deterioration of the results as the matrix size is increased. In fact, the accuracy increases as the size of the matrix to which the algorithm is applied is made larger. This outcome can be understood as follows: We will limit ourselves to the problem of detection of a and b, as a similar analysis holds true in the case of a' and b'. If a and b are estimates for the extreme eigenvalues of

$S_p(M)$, we have

$$\sup_{z\in S_p(M)} |P_n(z)| \leq \sup_{z\in[a,b]} |P_n(z)|. \tag{5.1}$$

Hence, with reference to (3.6), the larger the discrepancy in (5.1) the larger the error becomes in detecting a and b. However if the matrix is large (and if there are many distinct eigenvalues) then equality is essentially restored in (5.1). Indeed, in the presence of many eigenvalues it is likely that (at least) one of these eigenvalues will be located very near a point where the modified Chebyshev polynomial $P_n(z)$ reaches its extrema. For a small matrix (or of any matrix with few distinct eigenvalues) that it may happen that none of the eigenvalues are located near a point where the polynomial $P_n(z)$ reaches its extrema in which case a significant discrepancy takes place between the left hand side and the right hand side of (5.1). With regard to why the algorithms still work well problems like those typified in *Problem II*, (*i.e.* few distinct eigenvalues): Recall that the external extreme eigenvalues $(-.8, .8)$ had been found before hand, and we chose the polynomial $\mathcal{P}_{2n}^{a,b}(x)$ in (2.3) so that in that case

$$\sup_{x\in[-b,-a]\cup[a,b]} |\mathcal{P}_{2n}^{a,b}(x)| = |\mathcal{P}_{2n}^{a,b}(0.8)|. \tag{5.2}$$

(Also equal to $|\mathcal{P}_{2n}^{a,b}(-0.8)|$.) Hence we have equality between the sup in (5.2) and

$$\sup_{x\in Sp(M)} |\mathcal{P}_{2n}^{a,b}(x)|.$$

(Because 0.8 is in $Sp(M)$.) Deterioration take place if

$$\sup_{x\in[-b,-a]\cup[a,b]} |\mathcal{P}_{2n}^{a,b}(x)| \gg \sup_{x\in Sp(M)} |\mathcal{P}_{2n}^{a,b}(x)|.$$

6. Concluding Remarks. Finding the outer extreme eigenvalues, particularly of a Hermitian (or normal) matrix, is easily accomplished by traditional means, such as by the power method. Inverse iteration may be used to find inner extreme eigenvalues, however, it requires solving a linear system on every iteration. The reverse Chebyshev acceleration strategy for finding pairs of inner extreme eigenvalues is an effective alternative. The computational complexity of the methodology is $\mathcal{O}(m^2)$ for general dense Hermitian matrices. Theoretical estimates and numerical experiments were used to show that the scheme is numerically stable with respect to the size m of the matrix and thus viable even when the matrix is very large.

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Appendix A. Localization of the Outer Extreme Eigenvalues.

In what follows we assume that $-1 < a < b < 1$. The goal here is to define a minimum interval $[a, b]$ that contain all of the eigenvalues of M. The following theorem tells us whether a given interval has this property.

THEOREM A.1. *Let $-1 < s < r < 1$. Let the first guess x_0 be the eigenfunction associated with the largest eigenvalue and $e_0 = x_0 - x$. Let y_n be as described in (3.2), where the coefficients γ_k are those of $\tilde{P}_n^{s,r}(x)$. Then all the eigenvalues of M are located in $[s, r]$ if and only if*

$$\|y_n - x\| = \sup_{z\in[s,r]} |\tilde{P}_n^{s,r}(z)| \, \|e_0\|, \tag{A.1}$$

and

$$\tilde{P}_n^{s,r}(z) := \frac{P_n^{s,r}(z)}{P_n^{s,r}(1)}, \tag{A.2}$$

where $P_n^{s,r}(r) = 1$, $P_n^{s,r}(\lambda) > 1$ if $\lambda > r$.

Proof. Assume $S_p(M) \subset [s, r]$. Then in view of (3.6) we see that (A.1) holds.

Without loss of generality assume that one of the eigenvalues of M, say, λ is such that $\lambda > r$. Assume also, without loss of generality, that $1 - r > s + 1$ so that

$$\sup_{z\in[s,r]} |\tilde{P}_n^{s,r}(z)| = \tilde{P}_n^{s,r}(r) = \frac{1}{P_n^{s,r}(1)}.$$

Then we have, again in view of (3.6)

$$\|y_n - x\| = \sup_{z\in[s,\lambda]} |\tilde{P}_n^{s,r}(z)|\ \|e_0\|. \tag{A.3}$$

(We remark at this point that y_n is uniquely defined.) However, because $\lambda > r$,

$$\sup_{z\in[s,\lambda]} |\tilde{P}_n^{s,r}(z)| = \tilde{P}_n^{s,r}(\lambda) > \frac{1}{P_n^{s,r}(1)} = \sup_{z\in[s,r]} |\tilde{P}_n^{s,r}(z)|.$$

This demonstrates that instead of obtaining equality in (A.1), $\|y_n - x\|$ is greater than the right hand side of that equation.

□

Theorem A.1 can be interpreted as follows: If $\|y_n - x\| > \sup_{z\in[s,r]} |\tilde{P}_n^{s,r}(z)|\ \|e_0\|$ then it must be the case that $[s, r]$ does not contain all the eigenvalues of M, i.e., for s to be an estimate of a and r and estimate of b. However Theorem A.1 does not indicate the extent to which $[s, r]$ must be enlarged in order to contain all the eigenvalues of M. Our next result precisely addresses this question. We assume that for every eigenvalue $t \in S_p(M)$ we have $s < t$.

THEOREM A.2. *Let $-1 \le s < r < 1$. Let the first guess x_0 be such that the error e_0 is the largest eigenvalue, in absolute value, of $P_n(M) = \sum_{k=0}^{n} \gamma_k M^k$. Assume, with the notation of Theorem A.1, that*

$$\|y_n - x\| > \sup_{z\in[s,r]} |\tilde{P}_n^{s,r}(z)|\ \|e_0\| =: acc, \tag{A.4}$$

so that there are eigenvalues t of M with $t > r$. Then the largest eigenvalue b of M is the largest real solution η of the following equation:

$$\left|\tilde{P}_n^{s,r}(\eta)\right| = \frac{\|y_n - x\|}{\|e_0\|}. \tag{A.5}$$

Proof. In view of Theorem A.1 we have for the largest eigenvalue b of M

$$\|y_n - x\| = \sup_{z\in[s,b]} |\tilde{P}_n^{s,r}(z)|\ \|e_0\|, \tag{A.6}$$

But

$$\sup_{z\in[s,b]} |\tilde{P}_n^{s,r}(z)| = \tilde{P}_n^{s,r}(b).$$

Hence the theorem follows. □

Theorem A.1 tells us that if we overestimate, that is if $S_P(M) \subset [s, r]$, then it must be the case that (A.1) holds. However, we do not know how to adjust the interval $[s, r]$ so that it encloses more closely $S_P(M)$. Theorem A.2, in contrast, tells us that if we underestimate, *i.e.*, that there are eigenvalues t of M with $t > b$, then, in addition to knowing that we underestimate, we obtain in one step the largest eigenvalue of M. The solution η of (A.5) is now found using (2.1) together with the defining relation (A.2).

Define

$$\delta := \frac{\|y_n - x\|}{\|e_0\|} P_n^{s,r}(1). \tag{A.7}$$

We remark that the solution x is *fixed* (and known) throughout the procedure hence the dependence of δ on x is not indicated. Then, with η defined by (A.2) we introduce $\hat{y}$ satisfying

$$\eta = \frac{1}{2}(r-s)\tilde{y} + \frac{1}{2}(r+s) \tag{A.8}$$

or

$$\tilde{y} = \frac{1}{2}\left(\left(\delta + \sqrt{\delta^2-1}\right)^{\frac{1}{n}} + \left(\delta - \sqrt{\delta^2-1}\right)^{\frac{1}{n}}\right). \tag{A.9}$$

If there are eigenvalues t of M with $t < s$, then Theorem A.2 gives (in one step) the smallest eigenvalue of M. More precisely, an estimate η of the smallest eigenvalue is found by the above procedure, with (A.8) replaced by

$$\eta = -\frac{1}{2}(r-s)\tilde{y} + \frac{1}{2}(r+s), \tag{A.10}$$

(A.7) and (A.9) remaining unchanged. Indeed, the right hand side of (A.10) is the point symmetrically located with respect to $\frac{s+r}{2}$ of the right hand side of (A.8). The observed convergence $\|y_n - x\|$ is known.

A.1. The Outer Eigenvalue Algorithm. In order to determine the smallest interval containing all the eigenvalues of M we exploit Theorem A.1 and Theorem A.2.

Defining s and r as estimates of the outer eigenvalues a and b, respectively, we proceed as follows:

To estimate b:

1. choose $s = -1$ and make a guess for r, with $-1 < r < 1$. If (A.1) holds then all the eigenvalues of M are in $[s, r]$.
2. Choose $t < r$ and put $r \leftarrow t$. If (A.4) holds it must be the case that some eigenvalues of M are not contained $[s, r]$. Because $s = -1$, the eigenvalues of M not contained in $[s, r]$ are in fact larger than r.
3. Next, compute η using using (A.7), (A.8) and (A.9). and put $r \leftarrow \eta$.
4. We know now that the eigenvalues of M are located in $[s, r]$ and that r is an estimate for b, the rightmost eigenvalue of M.

Next, we proceed with the estimate of a:

5. choose $t > s(= 1)$ and put $s \leftarrow t$.
6. If (A.1) holds then all the eigenvalues of M are located in $[s, r]$.
7. If (A.4) holds then it must be the case that some eigenvalues of M are not located in $[s, r]$. These eigenvalues must be such that they are smaller than s because r is (an estimate for) the largest eigenvalue. Next, compute η as given by (A.7), (A.10) and (A.9) and put $s \leftarrow \eta$.
8. The interval $[s, r]$ is an estimate, within machine accuracy, of $[a, b]$.